

Supporting information.

Test and Evaluation of *ff99IDPs* Force Field for Intrinsically Disordered Proteins

Wei Ye,¹ Dingjue Ji,¹ Wei Wang,¹ Ray Luo,^{2,*} and Hai-Feng Chen^{1,3,*}

¹State Key Laboratory of Microbial metabolism, Department of Bioinformatics and Biostatistics, College of Life Sciences and Biotechnology, Shanghai Jiaotong University, 800 Dongchuan Road, Shanghai, 200240, China

²Departments of Molecular Biology and Biochemistry, Chemical Engineering and Materials Science, Biomedical Engineering, University of California, Irvine, California 92697-3900, USA

³Shanghai Center for Bioinformation Technology, 1278 Keyuan Road, Shanghai, 200235, China

*Corresponding authors

Email addresses: haifengchen@sjtu.edu.cn; ray.luo@uci.edu

Tel: 86-21-34204348

Fax: 86-21-34204348.

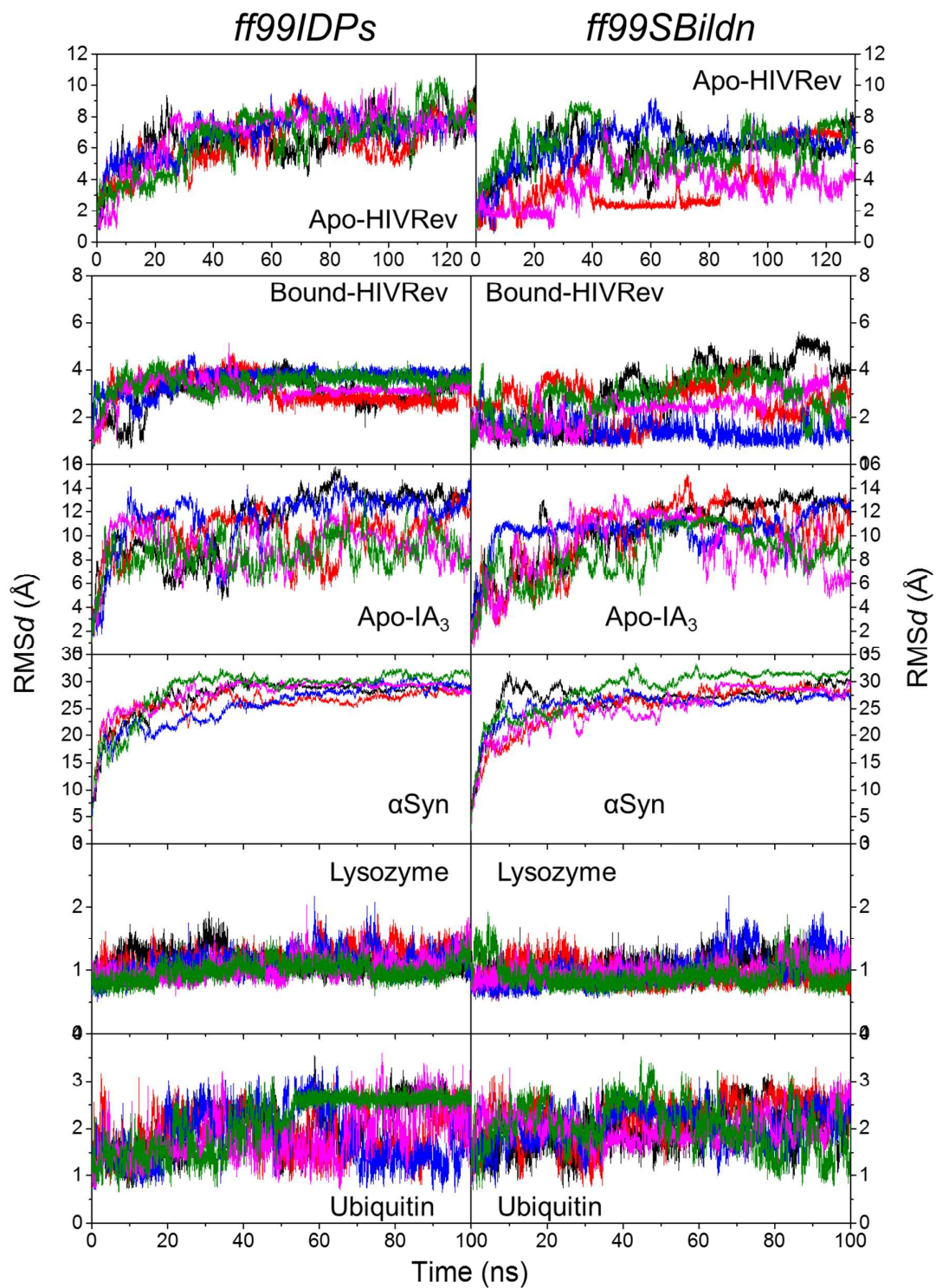


Figure S1. Time evolution of RMSd for all the simulated systems.

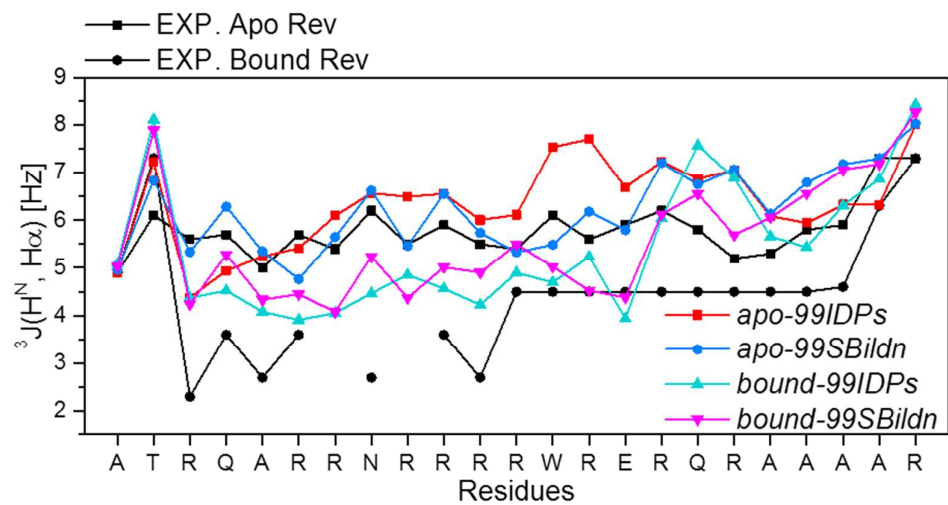


Figure S2. J-coupling of apo- and bound-HIVRev under both force field and their comparison with the experimental data.

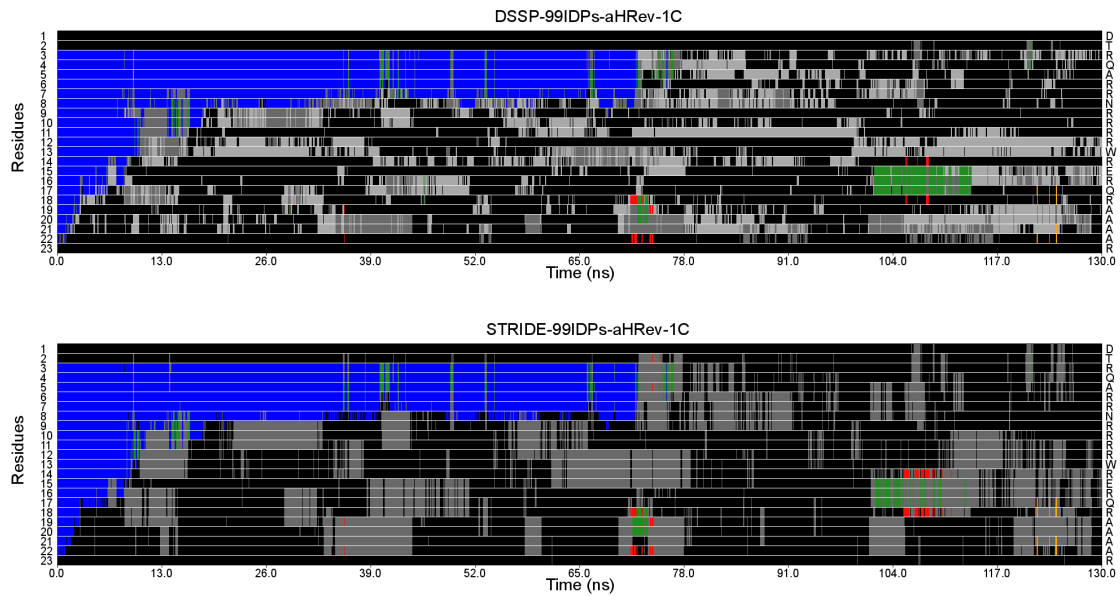


Figure S3. Comparison of secondary structure evolution between DSSP (top) and STRIDE (bottom) for apo-HIVRev under *ff99IDPs*. Colors labels: ■ α helix; ■ 3/10 helix; ■ π helix; ■ disordered loop; ■ bend; ■ hydrogen bonded turn; ■ extended strand; ■ residue in isolated β -bridge.

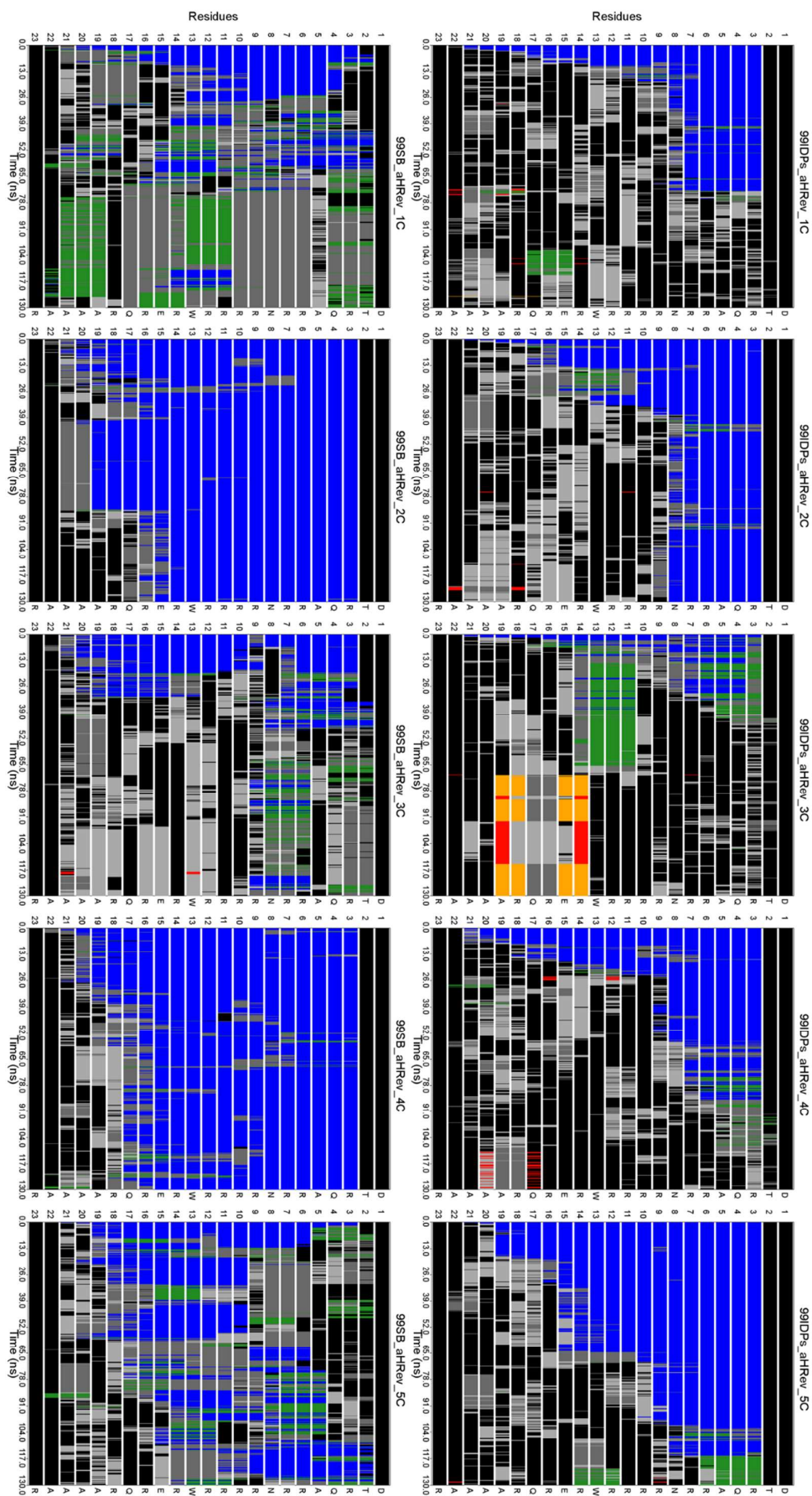


Figure S4. Time evolution of secondary structure for apo-HIVRev.

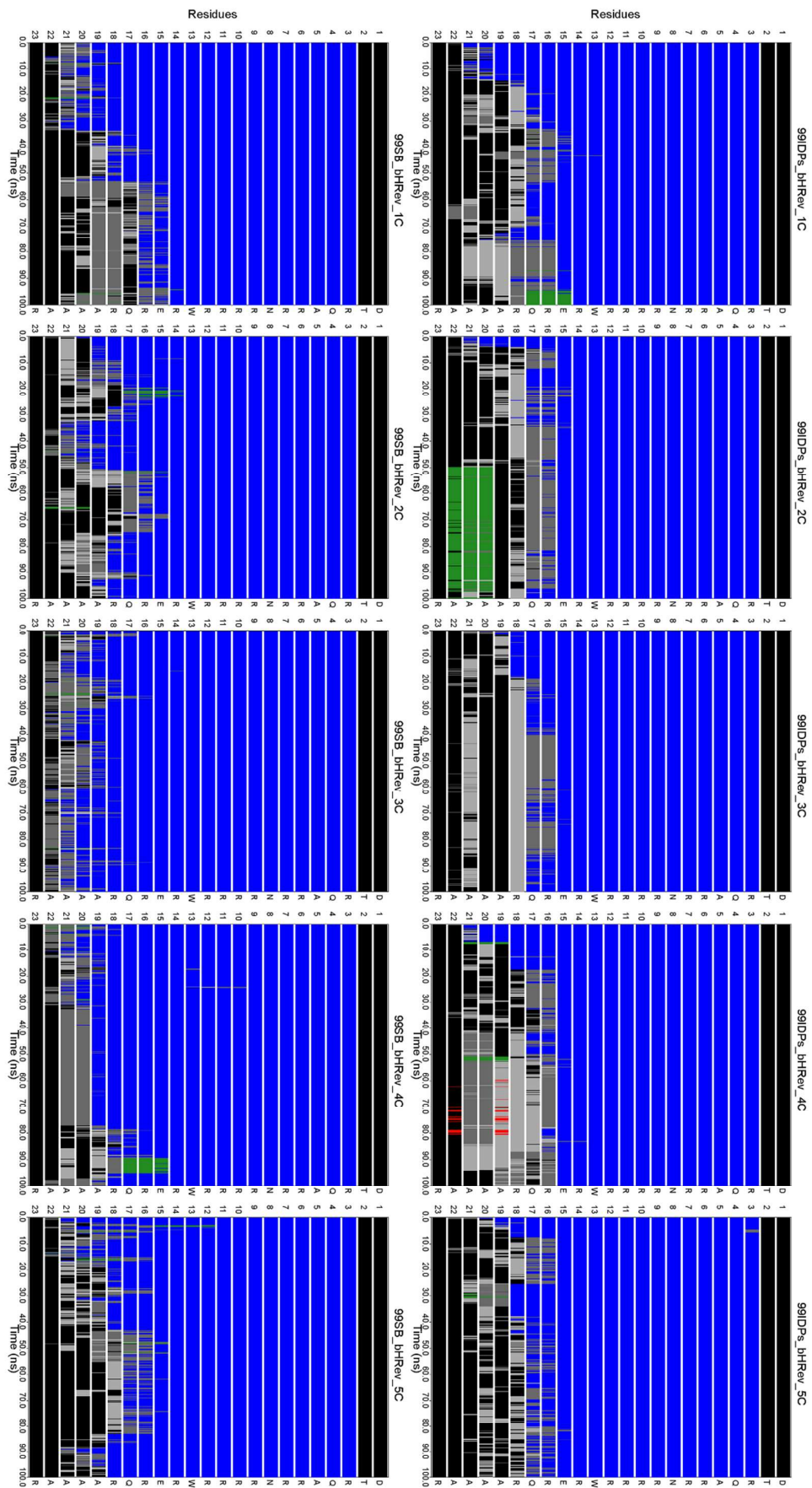


Figure S5. Time evolution of secondary structure for bound-HIVRev.

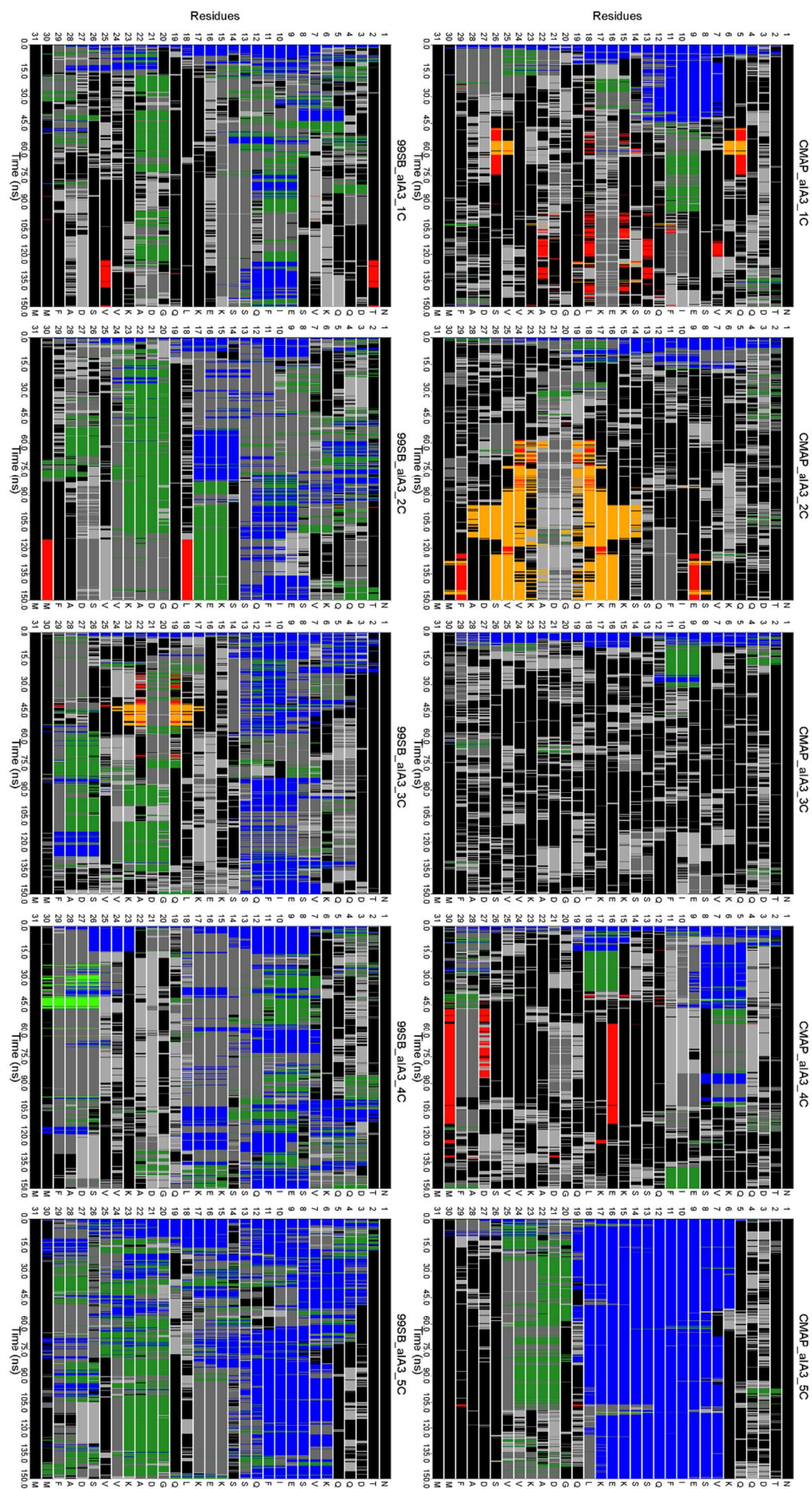


Figure S6. Time evolution of secondary structure for apo-IA₃.

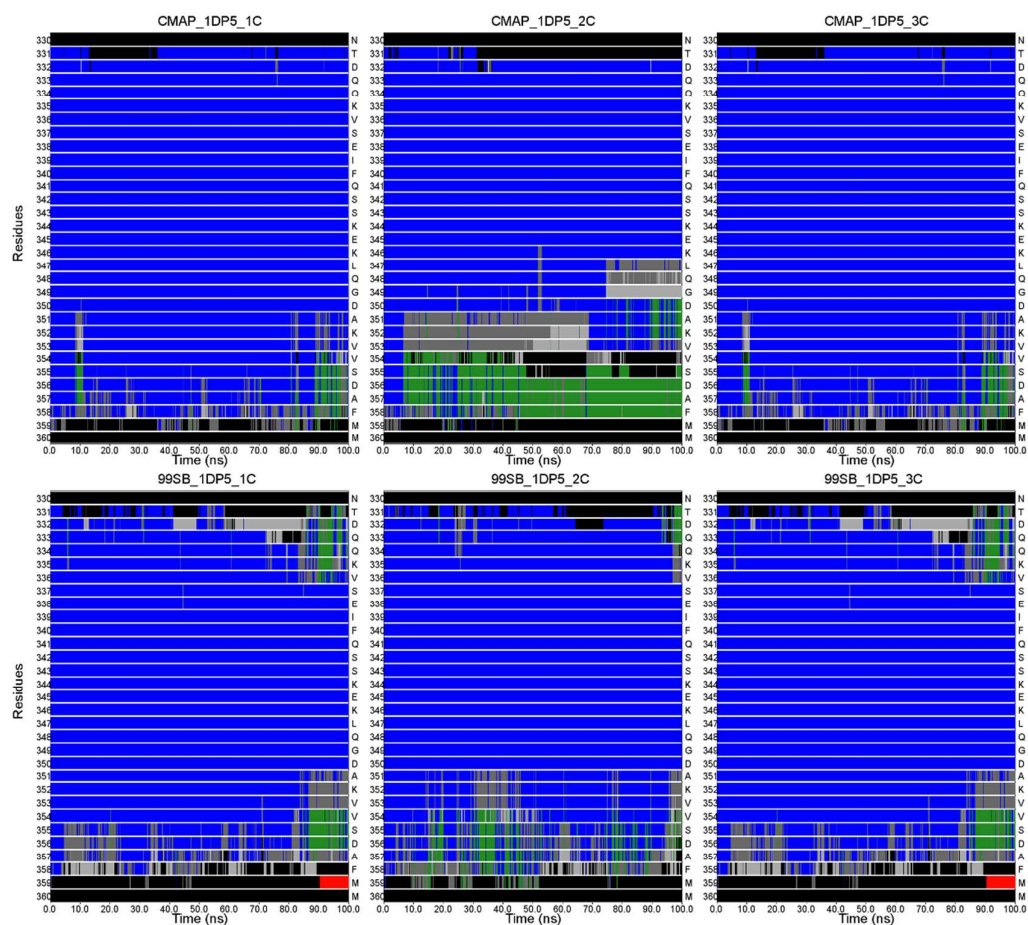


Figure S7. Time evolution of secondary structure for bound-IA₃.

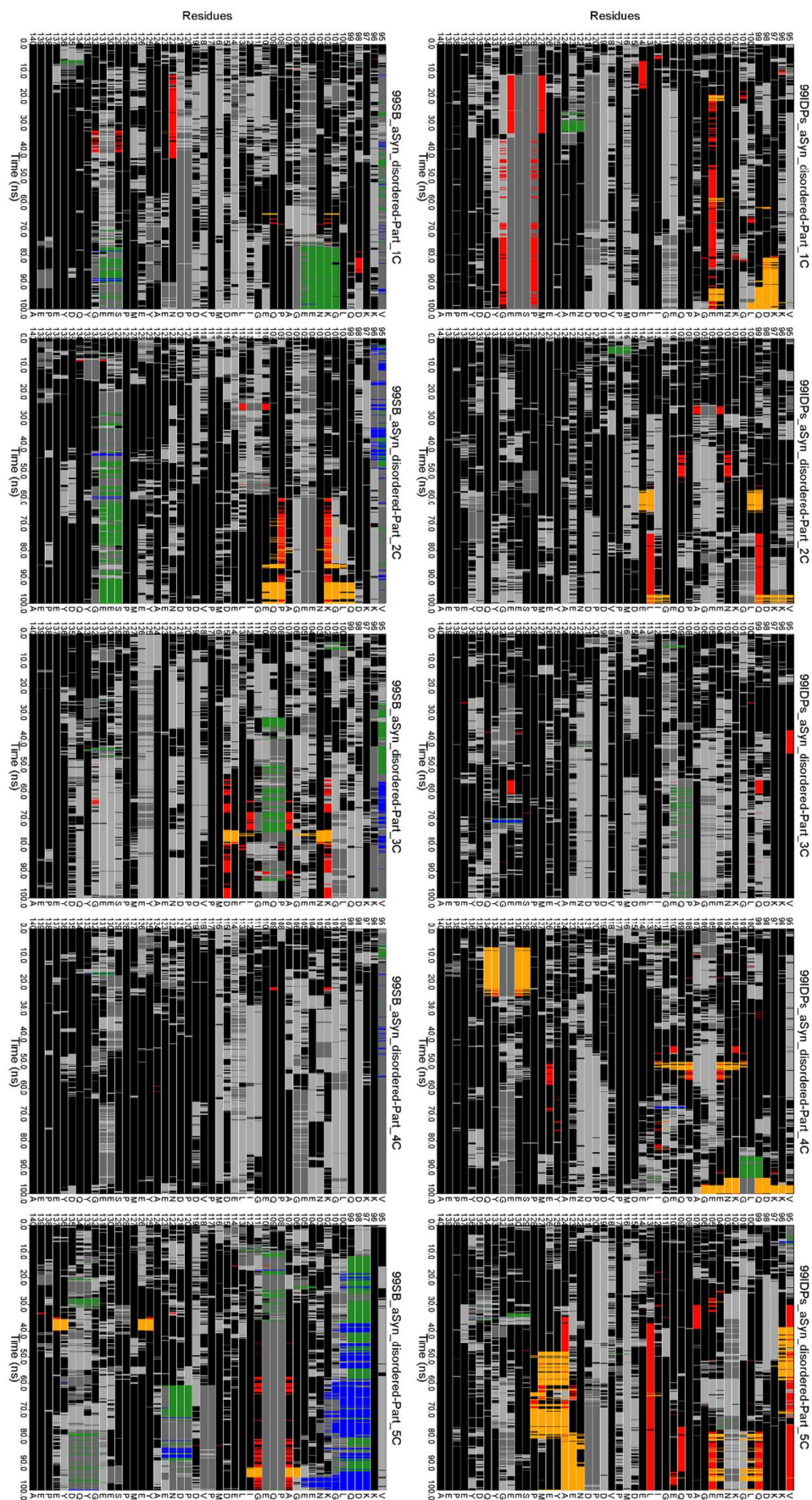


Figure S8. Time evolution of secondary structure for the disordered part of α Syn.

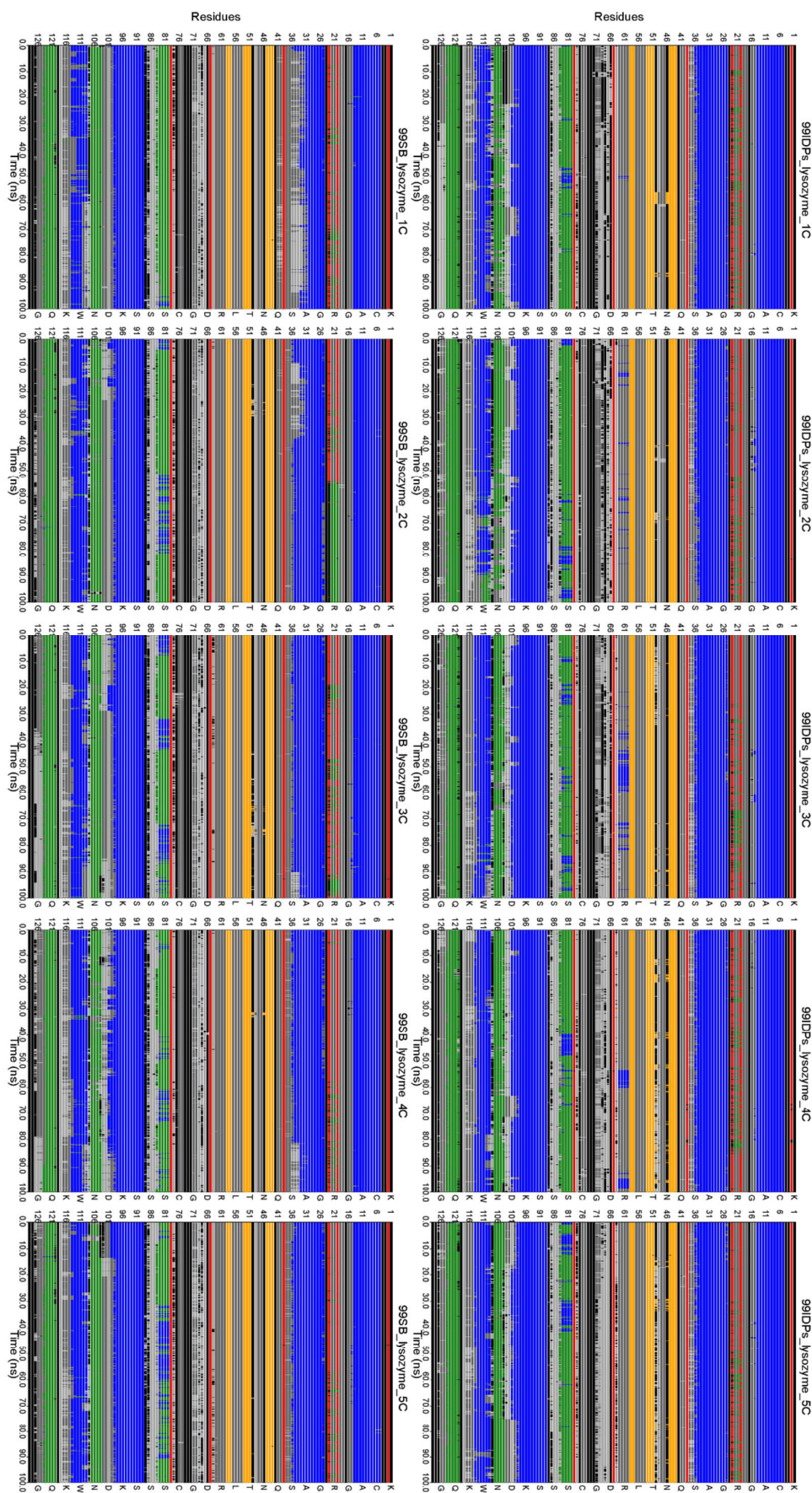


Figure S9. Time evolution of secondary structure for lysozyme.

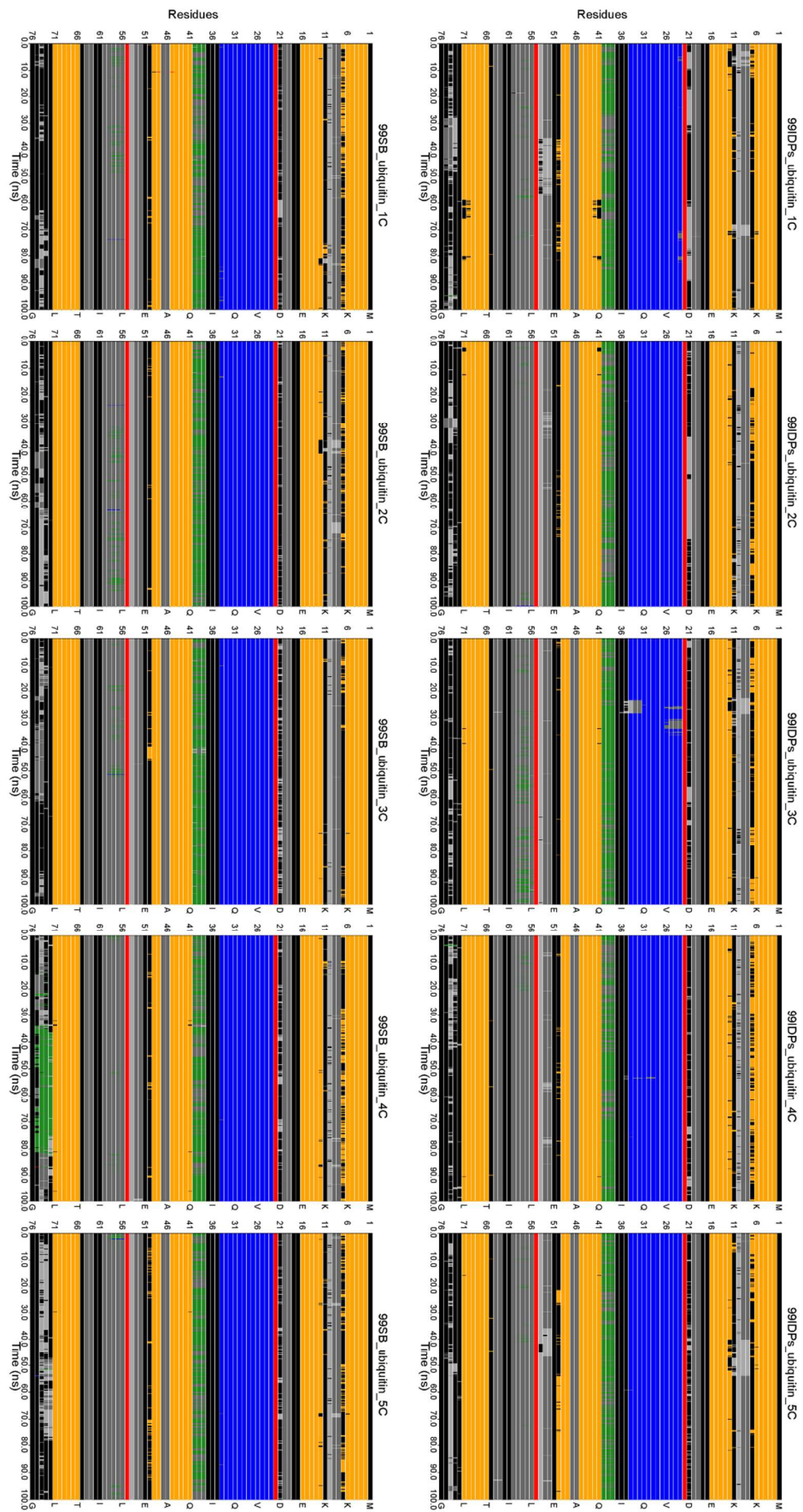


Figure S10. Time evolution of secondary structure for ubiquitin.

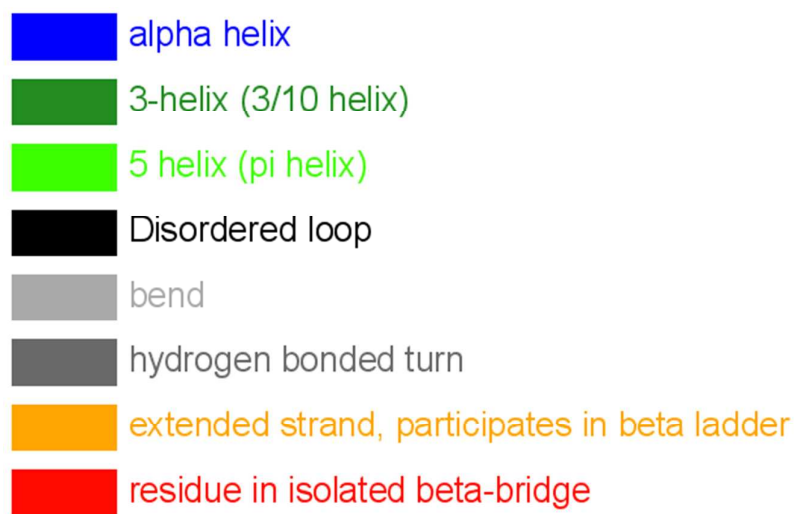


Figure S11. Color labels for different secondary structures.

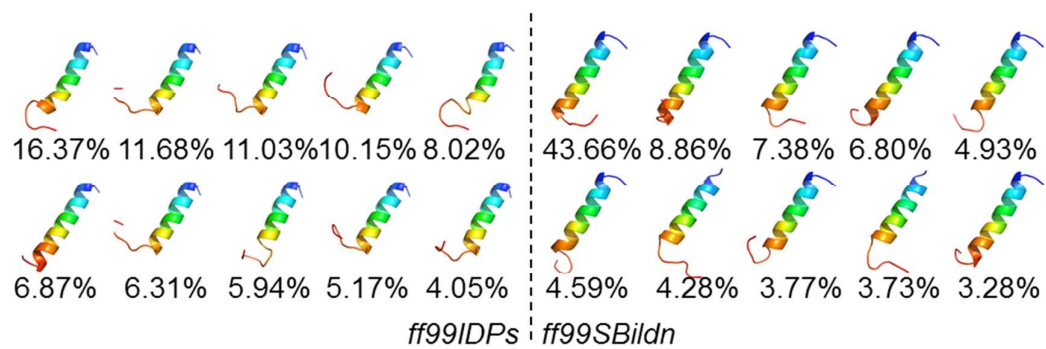


Figure S12. Structural clusters on bound HIVRev.

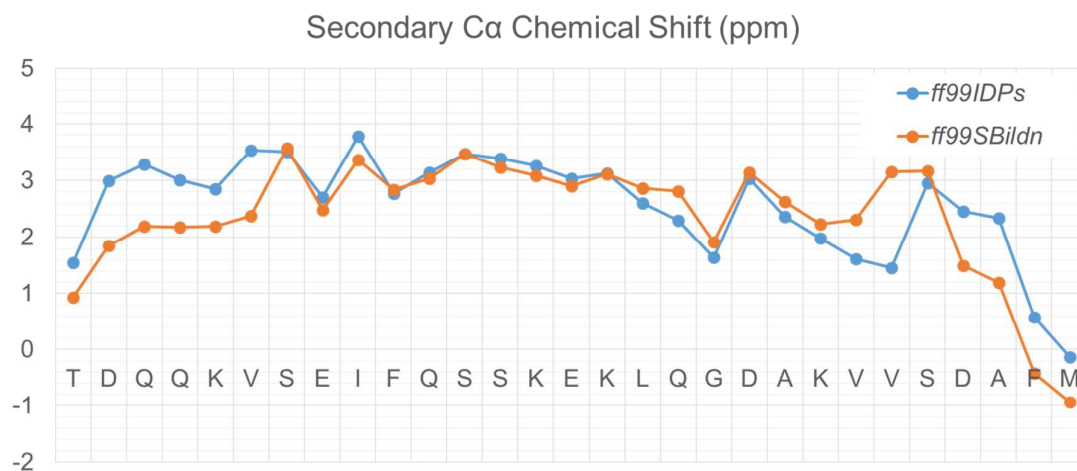


Figure S13. The predicted secondary chemical shift of bound-IA3 under ff99IDPs and ff99SBildn.